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MATHEMATICAL MODELING OF PROCESSES OF PULSED MELTING AND VAPORIZATION OF A METAL WITH CLEARLY SEPARATED PHASE BOUNDARIES

P. V. Breslavskii and V. I. Mazhukin

UDC 519.63-536.422.1

The authors propose a method of numerical solution of problems of the Stefan type with two moving boundaries. As an example they solve the problem of pulsed melting and vaporization of an aluminum rod of finite length.

The pulsed action of concentrated energy fluxes on an absorbing solid medium has been considered in a number of monographs [1, 2]. On the whole, however, this problem is far from being resolved, due to a number of specific special features. The main feature is that an increase of the energy density supplied above a specific value leads to the development of complex phenomena in the solid, associated with nonequilibrium states and phase transformations. The description of these processes theoretically encounters a number of difficulties of a physical and mathematical nature.

The physical difficulties arise from the absence at present of a complete theory of nonequilibrium phase transformations and the inadequacy of experimental data.

The mathematical difficulties are associated with the fact that in a pulsed action, e.g., on a metal, one must consider, as a rule, the thermophysical characteristics of the substance and the two phase transformations. Analytical solutions of this kind of nonlinear problem are known, but are more frequently the exception, and the main methods of solving them are finite-difference methods [3]. Usually phase transitions of type I are described in the approximation of the classical Stefan problem [4], for which the main difficulties of

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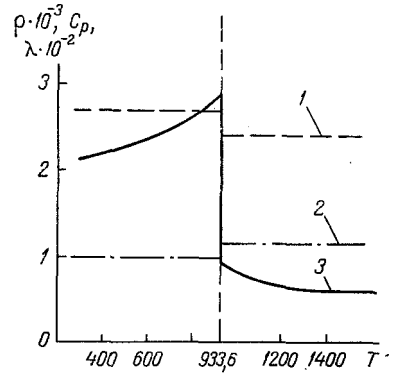

Fig. 1

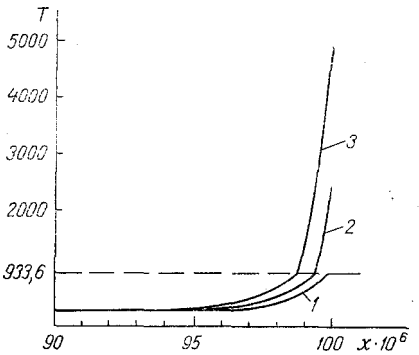

Fig. 2

Fig. 1. Temperature dependences: 1) $\rho(T)$; 2) $C_p(T)$; 3) $\lambda(T)$. T, K; ρ, kg/m^3; $C_p(T)$, kJ/(kg·deg); λ, W/(m·deg).

Fig. 2. Spatial temperature profiles at different times: 1) $t = -30.76\cdot10^{-9}$ sec; 2) $-16.83\cdot10^{-9}$; 3) $6.96\cdot10^{-9}$ sec. x, m.

solution are due to the moving boundaries of the phases. Two approaches have been used mostly in solving the Stefan problem: determining the classical solution with explicit separation of the phase boundaries [5, 6], and a generalized solution with the aid of a smoothing procedure in a straight-through computation [7, 8]. The use of straight-through algorithms is most efficient in solving multidimensional problems [9, 10]. Separation of the position of the fronts gives the most complete and detailed information on the ambient processes, and allows correct computation in the problem of the role of hydrodynamics effects, the volume energy source, and the lack of equilibrium of phase transitions in explicit form. However, numerical algorithms based on the principle of explicit separation of the phase front meet the nonsimple problem of adjusting the computing mesh, and as a rule are cumbersome and consume much machine time. Also, in most cases these algorithms are intended for solving problems with one phase front [11, 12]. It is therefore very important to develop economical and more sophisticated algorithms for solving problems concerning phase transitions of substances with explicitly separated phase boundaries, when the number of boundaries exceeds one. One approach to solving this problem may be the method of adaptive meshes, linked dynamically to the solution, as proposed by the authors of [13, 14].

In the present work the method of [13, 14] is generalized to the case of a problem with two moving phase fronts. As an example we solve the problem describing the processes of melting and vaporization of a metal rod of finite length exposed to the pulsed action of a heat source.

Statement of the Problem and Method of Solution. We formulate the unsteady spatially one-dimensional problem of melting and vaporization of a metal under the action of an energy flux with a gaussian distribution of intensity with time.

Description of the problem of phase transitions of the melting or solidifying type reduces to a nonlinear equation of heat conduction in a region with a previously unknown moving boundary $\Gamma_{s\ell}(T)$ separating the solid and liquid phases:

$$\rho_i(T)\,C_{pi}(T)\,\frac{\partial T_i}{\partial t}=\frac{\partial}{\partial x}\,\lambda_i(T)\,\frac{\partial T_i}{\partial x},\quad i=s,\ l. \tag{1}$$

At the phase interphase we have the Stefan differential condition

$$\lambda_s\,\frac{\partial T_s}{\partial x}-\lambda_l\frac{\partial T_l}{\partial x}=\rho_s v_{sl}L_m. \tag{2}$$

Besides Eq. (2) at the phase boundary we also assign a condition associated with the kinetics of the phase transition. In the classical variant of the Stefan problem used to describe the processes of melting or solidification it is ordinarily assumed that the temperature is continuous at the phase interface

$$T_s=T_l=T_m \tag{3}$$

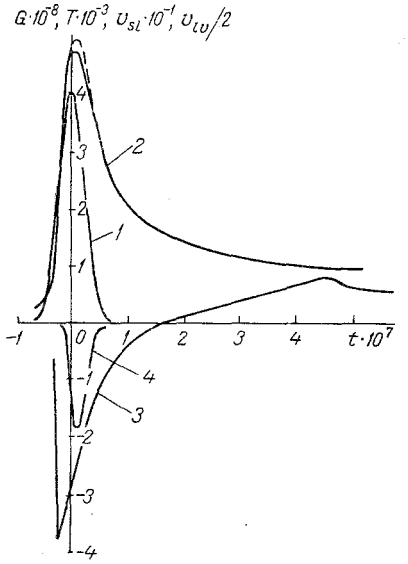

Fig. 3

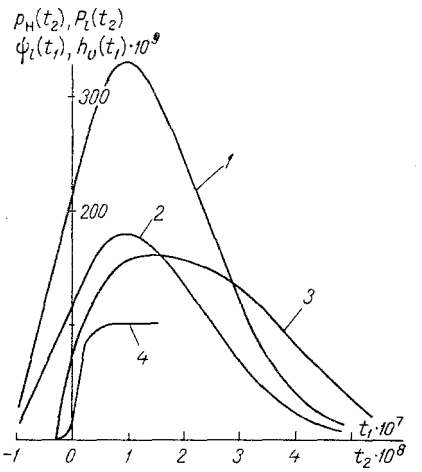

Fig. 4

Fig. 3. Timewise dependences: 1) G(t); 2) T(t) (the solid line is the Hertz–Knudsen formula, and the broken line is the Knudsen layer approximation); 3) $v_{S\ell}(t)$; 4) $v_{\ell V}(t)$. G, kW/m^2; T, K; $v_{S\ell}$, $v_{\ell V}$, m/sec; t, sec.

Fig. 4. Timewise dependences: 1) $p_H(t_2\cdot10^{-8})$; 2) $P_\ell(t_2\cdot10^{8})$; 3) $\psi_\ell(t_1\cdot10^{-7})$ (to determine the thickness of the liquid phase we used the formula $h_\ell = 1.61\cdot10^{-8}\ \psi_\ell$); 4) $h_V(t_1\cdot10^{-7})$. t_2, t_1, sec; p_H, P_ℓ, bar; H_V, m.

and is equal to the equilibrium transition temperature T_m which in many cases can be regarded as constant.

The vaporization process is a transition of the material from the condensed state to the gaseous, and compared with melting has a large specific heat and a large specific volume. Vaporization of metals by concentrated energy fluxes in the subcritical temperature region, where there is a clearly pronounced liquid-vapor boundary, can occur in two substantially different regimes. In one of these the gasdynamic perturbations in the flow of vaporized material have no influence on the vaporization process [2], and in the second the gasdynamic factor can have a governing role [15, 16].

To describe the process of vaporization on the phase interface surface $\Gamma_{\ell V}(t)$ we use the laws of conservation of mass, momentum and energy:

$$\rho_l v_{lv} = \rho\,(u - v_{lv}),\ P_l + \rho_l v_{lv}^2 = p + \rho\,(u - v_{lv})^2,$$
$$\lambda_l \frac{\partial T_l}{\partial x} = L_v \rho_l v_{lv} - G, \tag{4}$$

and also we formulate certain additional relations governing the kinetics of the phase transition. The simplest example of such a relation is the formula of the Hertz–Knudsen type:

$$J = \rho_l v_{lv} = \frac{p_H(T_l)}{(2\pi R T_l)^{1/2}}. \tag{5}$$

Equation (5) refers to the limiting case when one can neglect collisions in the gas phase near the interface. When this is not true one must take account of the flux of particles returning to the surface from the gas phase [2]. The value of the reverse flow is determined by the conditions of gasdynamic flight beyond the limits of the Knudsen layer, and a number of approximations are used to evaluate this numerically [2, 17, 18].

In pulsed action, depending on the ratio of the source parameters, we find vaporization regimes with subsonic speed. In the framework of our problem it was assumed that in the time interval considered the rate of vaporization was equal to the speed of sound.

Numerical solution of the problem of Eqs. (1)-(9) was accomplished with the aid of a finite-difference method in an adaptive mesh dynamically linked to the solution [14, 15].

The method of [14, 15] is based on the idea of an automatic coordinate transformation with the help of the desired solution, which allows us to free ourselves from the moving boundaries and adjust the computing mesh at each time step. The determination of the mesh functions and the coordinate nodes are then continuously linked. The close interconnection is reduced to the level of a differential model, in general a nonlinear system of differential equations in partial derivatives. In this system some of the equations describe the phenomena under direct examination, and some describe the dynamics of the computing mesh, determined by the behavior of the desired solution.

We use a coordinte transformation of general type relevant to the case of the one-dimensional problem of Eqs. (1)-(5), with the aid of the substitution of variables: $x = \xi(q, t)$ is the forward transformation; and $q = \varphi(x, t)$ is the inverse transformation. Using these we can write

$$x = \xi(\varphi(x, t), t). \tag{6}$$

We differentiate Eq. (6) with respect to t, bearing in mind that x does not depend on t:

$$0 = \frac{\partial \xi}{\partial q}\frac{\partial \varphi}{\partial t} + \frac{\partial \xi}{\partial t} \quad \text{or} \quad 0 = \frac{\partial x}{\partial q}\frac{\partial q}{\partial t} + \frac{\partial x}{\partial t}.$$

Then $\frac{\partial q}{\partial t} = -\frac{\partial x}{\partial t} \Big/ \frac{\partial x}{\partial q}$. We introduce the notation:

$$\frac{\partial x}{\partial t} = -\frac{Q_i}{\rho_i}, \qquad \frac{\partial x}{\partial q} = \frac{\psi_i}{\rho_i}, \quad i = s, l. \tag{7}$$

Using Eq. (7) we have $\partial q/\partial t = Q_i/\psi_i$, and in addition we have

$$H(x, t) = H(\xi(q, t), t) = \tilde{H}(q, t), \quad W(x, t) = W(\xi(q, t), t) = \tilde{W}(q, t),$$

$$\frac{\partial H}{\partial t} = \frac{\partial \tilde{H}}{\partial q}\frac{\partial q}{\partial t} + \frac{\partial \tilde{H}}{\partial t} = \frac{\partial \tilde{H}}{\partial t} + \frac{Q}{\psi}\cdot\frac{\partial \tilde{H}}{\partial q}, \quad H = \rho(T) C_p(T) T,$$

$$\frac{\partial W}{\partial x} = \frac{\partial \tilde{W}}{\partial q}\frac{\partial q}{\partial x} = \frac{\rho}{\psi}\frac{\partial \tilde{W}}{\partial q}, \quad W = -\lambda(T)\frac{\partial T}{\partial x}.$$

The heat conduction equation (1) in variables q and t has the form

$$\frac{\partial \tilde{H}_i}{\partial t} + \frac{Q_i}{\psi_i}\frac{\partial \tilde{H}_i}{\partial q} = -\frac{\rho_i}{\psi_i}\frac{\partial W_i}{\partial q}, \quad i = s, l.$$

The second equation, which is the continuity equation, we obtain from Eq. (7) by differentiating it with respect to t:

$$\frac{\partial}{\partial t}\frac{\partial x}{\partial q} = \frac{1}{\rho_i}\frac{\partial \psi_i}{\partial t}, \quad \text{whence} \quad \frac{\partial \psi_i}{\partial t} = -\frac{\partial Q_i}{\partial q}.$$

Putting the heat conduction equation in divergent form and omitting the tilda sign, we write the problem of Eqs. (1)-(5) in the computing space in the final form:

$$\frac{\partial (\psi H)_i}{\partial t} = -\frac{\partial W_i}{\partial q} - \frac{\partial (QH)_i}{\partial q}, \quad i = s, l, \tag{8}$$

$$\frac{\partial W_i}{\partial t} = -\frac{\partial Q_i}{\partial q}, \tag{9}$$

$$\frac{\partial x}{\partial q} = \frac{\psi_i}{\rho_i}. \tag{10}$$

In these variables Eq. (8) is the energy balance equation, Eq. (9) is the continuity equation describing the law of conservation of mass, and Eq. (10) is the equation connecting the variables x and q.

Choice of the Function Q. The function Q ensures a specific form of coordinate transformation. In general its structure is arbitrary and must be determined by the special

features of the solution which naturally predetermine the use of adaptive meshes in the computations. A special feature of solving the Stefan problem, as has been mentioned, is the presence of a continuously varying region. The construction of the adaptive mesh for such a region consists in the simplest case of an equation for the distribution of nodes, close to equilibrium at each time instant. One can achieve this kind of distribution by assigning a function Q in the form of the diffusion flux $Q=-D\frac{\partial\psi}{\partial q}$ where D is the diffusion coefficient (in the simplest cases we can take it as constant). In our work D was expressed in terms of the thermophysical characteristics of the medium: $D = \rho^2\lambda/C_p\psi$.

Boundary Conditions. The boundary conditions for Eqs. (8) and (9) are formulated as follows. On the solid-liquid interface ($q = q_{s\ell} = \Gamma_{s\ell}$) for the heat conduction equation we use Eq. (3)

$$T_s(\Gamma_{sl},\ t) = T_l(\Gamma_{sl},\ t) = T_m.$$

The condition for Eq. (9) is written in the form of a flux of material through the phase boundary $Q_{s\ell}$ whose value is determined from condition (2): $Q_{s\ell} = -(W_s - W_\ell)/L_m$.

At the left boundary on the solid side $q = q_0$ and there can be any boundary conditions for the heat conduction equation. Because there is no flux of material through the boundary for the continuity equation the boundary condition has the form $Q(q_0, t) = 0$. At the moving liquid—vapor boundary ($q = q_{\ell v} = \Gamma_{\ell v}$) the flux of material is not zero and the boundary conditions for Eqs. (8) and (9) are determined from Eqs. (4) and (5)

$$\frac{\lambda\rho_l}{\psi_l}\frac{\partial T_l}{\partial q} = L_v Q_{lv} - G.$$

The flux $Q_{\ell v}(\Gamma_{\ell v}, t)$ was determined by two methods: without allowing for the reverse flow, for which we used Eq. (5)

$$Q_{lv}(\Gamma_{lv},\ t) = \rho_l v_{lv} = \frac{p_н(T_l)}{(2\pi RT_l)^{1/2}},$$

and allowing for the flux of returning particles

$$Q_{lv}(\Gamma_{lv},\ t) = \rho(u - v_{lv}).$$

The velocity u was assumed equal to the sound speed: $u = (\gamma RT)^{1/2}$. The unknowns ρ and T were determined from the relations of [17].

Thus, the problem of moving phase boundaries in the computing space reduces to determining the fluxes $Q_{s\ell}$, $Q_{\ell v}$. To approximate the nonlinear system (8) and (9) we used a difference scheme written with the aid of the integrointerpolation method:

$$\begin{gathered}\frac{(\psi H)^{J+1}_{i+1/2} - (\psi H)^{J}_{i+1/2}}{\tau} = -\frac{W^{J+1}_{i+1} - W^{J+1}_{i}}{h_{i+1/2}} - \frac{(QH)^{J+1}_{i+1} - (QH)^{J+1}_{i}}{h_{i+1/2}},\\ \frac{\psi^{J+1}_{i+1/2} - \psi^{J}_{i+1/2}}{\tau} = -\frac{Q^{J+1}_{i+1} - Q^{J+1}_{i}}{h_{i+1/2}},\\ \frac{x^{J+1}_{i+1} - x^{J+1}_{i}}{h_{i+1/2}} = \frac{\psi^{J+1}_{i+1/2}}{\rho^{J+1}_{i+1/2}}.\end{gathered} \tag{11}$$

To solve the system of nonlinear difference equations we used the method of matrix forward marching with iterations for nonlinearity [19]. The difference scheme (11) was solved in each phase subregion; in the solid phase we chose a nonuniform mesh with number of cells $N_s = 30$, and in the liquid phase we chose a uniform mesh with $N_\ell = 19$.

Results of Modeling. We consider the problem of melting and vaporization of a condensed medium with thermophysical properties typical for aluminum [20] (Fig. 1). The energy source was chosen to have parameters typical of concentrated energy sources: $G = G_0 \exp(-t^2/\tau^2)$, $\tau = 3\cdot10^{-8}$ sec, $G_0 = 4\cdot10^8$ kW/m^2. One topic of the investigation was to determine the role of the kinetic vaporization condition used, Eq. (5) [17], in solving the problem as a whole. The results of the modeling are presented in Figs. 2-4.

The calculations show that melting arises at time $t = -3.076\cdot10^{-8}$ sec (Fig. 2). The phase separation boundary in the spatial and timewise temperature profiles T(x), T(t) is

defined by the knee of the curves (Figs. 2, 3). The characteristic speeds of motion of the melt front reach tens of meters per second (Fig. 3). The positive branch of the curve $v_{s\ell}(t)$ corresponds to the crystallization process, and the negative branch corresponds to melting. The maximum depth of the liquid phase is reached at time $t = 1.28 \cdot 10^{-7}$ sec and is equal to $L_\ell \approx 2.6$ μm (Fig. 4). Vaporization occurs at any temperature, but at low temperatures the rate of vaporization is exceedingly small, and a noticeable motion of the phase boundary begins when $v_{\ell v}$ reaches several centimeters per second. The maximum speed of motion of the vaporization front $v_{\ell v}$ is almost an order of magnitude less than the speed $v_{s\ell}$ (Fig. 3), and correspondingly the thickness of the vaporized layer is much less than that of the melt (Fig. 4), and reaches 0.1 μm.

The numerical experiment has shown that one obtains very similar results by using one of the expressions of Eq. (5) or one of those given in [17, 18] as the kinetic vaporization condition. A comparison of the results using the Hertz–Knudsen formula, Eq. (5) (broken line) and using the condition from [17] (solid lines) is made in Fig. 3. If one computes the reflected flux of material using the relations of [17] one obtains comparatively noticeable differences in the values of the speed of motion of the vaporization front $v_{\ell v}$ and values of the surface temperature, since a smaller value of the rate of removal of material leads to larger values of surface temperature (Fig. 3). However, the differences observed in determining the outflow pressure P_ℓ, which, as is known, is one of the most sensitive and informative characteristics of the vaporization process, are not appreciable. When Eq. (5) is used we find $P_\ell = 0.5\ p_H$. In the model with the Knudsen layer [17] $P_\ell = 0.55\ p_H$ (Fig. 4). Thus, in the vaporization regimes with M = 1 one can use any of the models from Eq. (5) or [17, 18].

The dynamics of the computing mesh in each subregion can be described with the aid of the quantity ψ measuring how often the initial dimensions of the computing cells were changed. In the solid phase region ψ_s can vary from 1, which corresponds to no change, to 0, which corresponds to complete transition of the region to the liquid phase. In the calculations the maximum variation of ψ_s was 0.8. In the liquid phase region ψ_ℓ varied from an arbitrarily small quantity to a value determined by the volume of the melted material. For the parameters chosen in the calculations ψ_ℓ is practically independent of the variable x, and Fig. 4 presents the dependence $\psi_\ell(t)$ which shows how often the liquid phase region was changed, and also the spatial mesh step size h_i.

We note that the computing algorithm for one-dimensional problems does not impose any restrictions on the number of phase boundaries, and in principle this can be any number.

NOTATION

x, coordinate; t, time; q, computing variable; ρ, C_p, λ, density, specific heat and thermal conductivity; L_m, L_v, heat of melting and vaporization; T_m, T_b, temperature of melting and vaporization; R, gas constant; ε, W, specific energy and heat flux; p_H, P_ℓ, saturation and outflow pressures; p, v, T, pressure, velocity and temperature; u, speed of the gas flow; u_c, speed of sound; γ, M, ratio of specific heats and Mach number; G, source intensity; ψ, Q, coordinate transformation function; Γ, phase interface; J, flux of material across the boundary. Subscripts: s, ℓ, solid and liquid phases; $s\ell$, ℓv, interphase boundaries; use of ρ, T, u, p with no subscripts means that the corresponding parameter refers to the gas phase.

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IDENTIFICATION OF HEAT TRANSFER BETWEEN THE CASTING AND THE MOLD IN INGOTLESS ROLLING

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UDC 536.24

A method is proposed for determining the heat flux inside a roll-mold on the basis of solution of the inverse heat-conduction problem by the gradient method.

The study of casting processes in a roll-type mold in order to select efficient production schemes entails the development of a set of mathematical models capable of predicting the thermal and thermal-stress states of equipment and products [1]. As is known [2, 3], the most important factor which affects solidification is heat transfer between the casting and the mold. At the same time, direct measurement of temperatures and heat fluxes on the mold surface is not possible because the transducers fail from thermal and mechanical loads [4]. It was proposed in [5] that the contact temperature be determined by means of a so-called natural thermocouple. Here, the contacting bodies themselves act as the thermoelectrodes. However, such a method is not sufficiently reliable and, moreover, does not permit consideration of the temperature distribution along the contact. Given these circumstances, it is best to obtain temperature measurements at internal points and to use inverse-problem methods to establish the thermal parameters on the contact surface [6].

A sketch of the equipment used for casting in a roll-type mold is shown in Fig. 1. Since the radius of the roll is considerably smaller than its length, we will assume that there is no heat transfer in the axial direction. Then the thermal problem for quasisteady operation of the roll is described as follows in cylindrical coordinates (ρ, φ) :

$$\bar{v}\frac{\partial T}{\partial \varphi}=\frac{1}{\rho}\frac{\partial}{\partial \rho}\left(\rho\frac{\partial T}{\partial \rho}\right)+\frac{1}{\rho^2}\frac{\partial^2 T}{\partial \varphi^2}, \tag{1}$$

$$0<\varphi<2\pi,\ \rho_0<\rho<1,$$

$$\left.\frac{\partial T}{\partial \rho}\right|_{\rho=\rho_0}=\frac{\alpha R}{\lambda}(T|_{\rho=\rho_0}-T_{\text{coo}}), \tag{2}$$

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